Level Density of a Bose Gas and Extreme Value Statistics

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We establish a connection between the level density of a gas of noninteracting bosons and the theory of extreme value statistics. Depending on the exponent that characterizes the growth of the underlying single-particle spectrum, we show that at a given excitation energy the limiting distribution function for the number of excited particles follows the three universal distribution laws of extreme value statistics, namely, the Gumbel, Weibull, and Fréchet distributions. Implications of this result, as well as general properties of the level density at different energies, are discussed.

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The level density is an essential quantity in determining the thermodynamic properties of closed quantum systems. In interacting many-body (MB) systems its computation is in general a difficult problem. The most common framework is a mean-field approximation, where a gas of independent (quasi-)particles moves in an average self-consistent potential. In this case, the energy of the gas is expressed as the sum of the occupied single-particle (SP) energies. The computation of the MB level density thus reduces to a combinatorial problem: counting the number of ways into which the energy can be distributed among the particles. The level density has been extensively studied in fermionic systems, where detailed experimental data exist at different excitation energies and quantum numbers (see, for some recent progresses in this field, Refs. [1,2]). In spite of the experimental breakthroughs of the 1990's and of the many interesting developments that followed, the case of bosonic systems is much less known. Studies of the spectral properties have concentrated on the low energy range of the spectrum of the condensate phase, where collective effects and interactions play a crucial role.

Our aim here is to compute, within an independent-particle approximation, the asymptotic properties of the MB level density $\rho_{\mathrm{MB}}(E, N)$ of a Bose gas as a function of the excitation energy E and the particle number N. We will first consider two extreme regimes that correspond to the quantum-degenerate and to the classical limits of the gas. The level density in these two extreme cases behaves quite differently as a function of energy. In the former case, where one takes the $N \to \infty$ limit first keeping the energy E finite, the level density $\rho_{\mathrm{MB}}(E, \infty)$ increases with energy in a stretched-exponential manner for large E. In contrast, in the classical limit where one keeps N finite and takes the large E limit, the level density increases with energy in a power-law fashion. This leads to a natural question: what happens in between these two extreme regimes where both E and N are large but finite? The main result of this Letter is to show that in this intermediate regime the level density displays a rich variety of scaling behaviors depending on the SP spectrum and has an interesting connection to the extreme value statistics (EVS) of independent random variables. These different behaviors have measurable consequences in other thermodynamic properties of the system, such as the entropy, or the specific heat.

To explore this intermediate regime, we stay close to the degenerate-gas limit and compute explicitly the effect of a finite number of bosons N on the level density. In this regime, in a given configuration of excitation energy E, only a fraction of the particles contribute to E, the rest remain in the ground state. However, the ground-state occupancy and, consequently, the number of excited bosons, fluctuate among different configurations belonging to the same excitation energy E. These fluctuations may be small or anomalously large depending on the SP spectrum. To obtain a quantitative estimate of these fluctuations, we compute explicitly the distribution of the number of excited particles for a fixed (but large) E. We will show that the fraction of configurations at excitation energy E with N or less excited bosons has a limiting distribution (when suitably rescaled) for large N and large E. Depending on the index ν that controls the growth of the SP number of states [cf. Eq. (9) below], three limiting distributions emerge, namely, the Gumbel, Weibull, and Fréchet distributions. Interestingly, precisely the same three limiting distributions characterize the EVS of independent random variables [3], a field that has seen a recent resurgence of interests [4].

Our work provides a link between two *a priori* unrelated fields, namely, the combinatorial problem associated with a noninteracting Bose gas and the EVS. Interestingly, the Gumbel distribution has been shown to emerge in the quantum interference patterns of Bose liquids [5]. We also believe that our results are of interest in different branches of physics (such as in the computation of black hole entropy [6]), mathematics, and computer science. For instance, it is well known that the computation of the level density of a Bose gas in a one-dimensional (1D) harmonic potential (equidistant SP spectrum) is directly related to the theory of partitions of an integer [7,8]. Hence our results also provide a link between the number partitioning problem [9] and the EVS, generalizing a theorem due to Erdös and Lehner [10] (see also [11,12]) which states that the number of summands in a random partition of an integer is asymptotically distributed with the Gumbel law.

We consider noninteracting bosons confined by some single-particle potential whose energy levels are ϵ_j, $j = 0, 1, 2, \ldots$. We set $\epsilon_0 = 0$ without loss of generality. Each configuration $\{n_j\}$ of the gas is characterized by an excitation energy $E = \sum_{j=1}^{\infty} n_j \epsilon_j$ and a total number of particles $N = \sum_{j=0}^{\infty} n_j$, where $n_j = 0, 1, 2, \ldots$ is the occupation number of the jth SP level in that configuration. The level density at excitation energy E of a gas of N bosons is given by

$$\rho_{\rm MB}(E, N) = \sum_{\{n_j\}} \delta\left(E - \sum_{j=1}^{\infty} n_j \epsilon_j\right) \delta\left(N - \sum_{j=0}^{\infty} n_j\right). \quad (1)$$

The number of excited bosons is simply $N_{\rm ex} = N - n_0 = \sum_{j=1}^{\infty} n_j$. Since $n_0 \geq 0$, it follows that $N_{\rm ex} \leq N$. Thus, if one just keeps track of only the excited bosons, it is an easy exercise to show that $\rho_{\rm MB}(E, N)$ in Eq. (1) can also be interpreted as the number of configurations with energy E and with $N_{\rm ex} \leq N$. Thus, when $N \to \infty$, $\rho_{\rm MB}(E, \infty)$ simply counts the total number of configurations at energy E.

A convenient way to express Eq. (1) is by means of an inverse Laplace transform

$$\rho_{\rm MB}(E, N) = \frac{1}{(2\pi i)^2} \int_{a-i\infty}^{a+i\infty} d\beta \int_{b-i\infty}^{b+i\infty} d\alpha e^{S(\alpha,\beta)}, \quad (2)$$

where

$$S(\alpha, \beta) = -\beta\Omega(\alpha, \beta) + \beta E - \alpha N \quad (3)$$

is the entropy,

$$\Omega(\alpha, \beta) = -\int d\epsilon \frac{\mathcal{N}(\epsilon)}{e^{\beta\epsilon - \alpha} - 1} \quad (4)$$

the grand potential of the gas, and

$$\mathcal{N}(\epsilon) = \int^{\varepsilon} \rho(\varepsilon) d\varepsilon \quad (5)$$

the integrated density of states expressed in terms of the SP density of states $\rho(\epsilon) = \sum_j \delta(\epsilon - \epsilon_j)$. In Eq. (2), a and b are real parameters such that all the poles of the integrand are to the left of the integration path.

A saddle point approximation with respect to the auxiliary parameters α and β of the integrals in Eq. (2) yields

$$\rho_{\rm MB}(E, N) = e^{S(\alpha,\beta)}/2\pi\sqrt{|\mathcal{D}(\alpha, \beta)|}, \quad (6)$$

where $\mathcal{D}(\alpha, \beta)$ is the determinant of the second derivatives of $S(\alpha, \beta)$. The dependence on N and E in Eq. (6) arises from the saddle point conditions that determine implicitly the values of α and β in terms of N and E

$$\mathcal{N}(\alpha, \beta) = \int d\epsilon \frac{\rho(\epsilon)}{e^{\beta\epsilon - \alpha} - 1} = N, \quad (7)$$

$$\mathcal{E}(\alpha, \beta) = \int d\epsilon \frac{\epsilon\rho(\epsilon)}{e^{\beta\epsilon - \alpha} - 1} = E, \quad (8)$$

where $\mathcal{N}(\alpha, \beta)$ and $\mathcal{E}(\alpha, \beta)$ are the particle number and energy functions of the gas, respectively. We will work here in the leading order approximation $\rho_{\rm MB}(E, N) \approx e^{S(\alpha,\beta)}$, and thus ignore the prefactor in Eq. (6).

In Eqs. (7) and (8) all the nontrivial information is contained in the SP level density $\rho(\epsilon)$. We use here the continuous approximation, in which the discreteness of the SP energy levels ϵ_j is ignored and $\rho(\epsilon)$ is replaced by a smooth function. We assume moreover that the high energy growth of the integrated density of states is well approximated, on average, by

$$\mathcal{N}(\epsilon) \approx \epsilon^{\nu}. \quad (9)$$

Here ϵ is an adimensional energy. To recover dimensional quantities in the formulas below, all energies must be multiplied by some appropriate factor κ. The index ν is a real positive number that can take arbitrary values depending on the confining potential. For instance, if the gas is trapped by a one-dimensional potential $V(x) \propto |x|^a$, with $a > 0$, then it simply follows from the WKB approximation that $\nu = (a + 2)/2a$. This corresponds to the fact that energy levels grow as $\epsilon_j = j^s$, where $s = 1/\nu$. More generally, when the confining potential is a D-dimensional harmonic oscillator, then $\nu = D$, while when it is a D-dimensional box (hard wall cavity potential), then $\nu = D/2$ (and, for instance, $\kappa = (V/6\pi^2)^{2/3}(2m/\hbar^2)$ when $D = 3$, where V is the volume of the cavity and m the mass of the particle).

From Eqs. (4) and (8), using (9) and, consequently, $\rho(\epsilon) = \nu\epsilon^{\nu-1}$, the energy and grand potential are simply related by $\mathcal{E}(\alpha, \beta) = -\nu\Omega(\alpha, \beta)$. The entropy (3) may thus be written, taking into account the condition (8),

$$S(\alpha, \beta) = (1 + 1/\nu)\beta E - \alpha N. \quad (10)$$

For any finite N, α is easily seen from Eq. (7) to be negative. A standard series expansion of the denominator in Eqs. (7) and (8) in terms of $z = \exp(\alpha)$, where $0 < z < 1$, allows us to write, in the continuous approximation, the two saddle point conditions as

$$\mathcal{N}(\alpha, \beta) = \frac{\Gamma(\nu + 1)}{\beta^{\nu}} {\rm Li}_{\nu}(z) = N, \quad (11)$$

$$\mathcal{E}(\alpha, \beta) = \frac{\nu\Gamma(\nu + 1)}{\beta^{\nu+1}} {\rm Li}_{\nu+1}(z) = E, \quad (12)$$

where ${\rm Li}_{\nu}(z) = \sum_{k=1}^{\infty} z^k/k^{\nu}$ is the polylogarithm function and Γ is Euler function.

Equation (11) shows that $\mathcal{N}(\alpha, \beta)$ is an increasing function of z. Therefore, when N increases at a fixed temperature $T = \beta^{-1}$, z needs to increase to satisfy the equality. As $N \to \infty$, $z \to 1$. In that limit, the energy is easy to obtain and we get $\mathcal{E}(0, \beta) = \nu \int_0^{\infty} d\epsilon \epsilon^{\nu}/[\exp(\beta\epsilon) - 1] = \theta_{\nu}/\beta^{\nu+1}$, where

$$\theta_{\nu} = \nu\Gamma(\nu + 1)\zeta(\nu + 1) \quad (13)$$

[$\zeta(z) = {\rm Li}_1(z)$ is the Riemann zeta function]. From Eq. (12), we obtain the following relation between inverse temperature and excitation energy,

$$\beta = \beta_\nu = [\theta_\nu / E]^{1/(1+\nu)}. \quad (14)$$

Using this expression for β and setting $\alpha = 0$ in Eq. (10), we get to leading order in a high energy expansion (i.e., large energies compared to the spacing between SP energy levels)

$$\rho_{\rm MB}(E, \infty) = \exp[(1 + 1/\nu)(\theta_\nu E^\nu)^{1/(\nu+1)}]. \quad (15)$$

For $\nu = 1$ this equation reproduces the well-known asymptotic result for an equidistant spectrum $\epsilon_j = j$ (1D harmonic potential), $\rho_{\rm MB}(E, \infty) = e^{2\sqrt{\pi^2 E/6}}$, obtained by Hardy and Ramanujan in the partition problem [13]. It was generalized to arbitrary 1D potentials $\epsilon_j \propto j^{1/\nu}$ (partitions into nonintegral powers of integers) in [14]. In the present context, Eq. (15) is valid for any system whose average counting function behaves (asymptotically) like Eq. (9) (see also Ref. [12]). For instance, it holds for a 3D harmonic potential ($\nu = 3$), or a 2D box of arbitrary shape (or billiard), ($\nu = 1$).

Equation (15) describes the density in the limit of an infinite number of particles for a large but finite excitation energy E. In the opposite limit, of a large excitation energy at a fixed number of particles, the density behaves quite differently. This is the Maxwell-Boltzmann limit, where the gas behaves classically. From Eq. (11), keeping N fixed and increasing the temperature (e.g., decreasing β), it follows that $z \to 0$ to satisfy the equality. Then ${\rm Li}_\nu(z) \approx z$ for any ν, and the stationary phase conditions (11) and (12) become $N = \Gamma(\nu + 1)z/\beta^\nu$ and $E = \nu\Gamma(\nu + 1)z/\beta^{\nu+1}$. The relation between temperature and excitation energy now is

$$E = \nu N T. \quad (16)$$

This simple equation generalizes, to an arbitrary confining potential, the well-known equipartition of energy valid for quadratic Hamiltonians. It provides a precise relation between a quantum spectral property (the index ν) and the partition of energy in the classical limit. From the previous form of the stationary phase conditions when $z \to 0$ we also get $\alpha = \log[\beta^\nu N/\Gamma(\nu + 1)]$. Using this relation for α and Eq. (16) for β in Eq. (10), the many-body level density now takes the form

$$\rho_{\rm MB}(E, N) = \left[\frac{\Gamma(\nu + 1)}{\nu^\nu} \frac{E^\nu}{N^{\nu+1}}\right]^N e^{(\nu+1)N}. \quad (17)$$

In contrast to Eq. (15), in the classical limit the level density has a power-law dependence on the excitation energy (similar results in some particular cases were obtained in [15], using different methods). When $E \gg N \gg 1$, using Stirling's approximation this equation may be written as

$$\rho_{\rm MB}(E, N) = \frac{[\Gamma(\nu + 1)]^N}{N!} \binom{E}{\nu N}.$$

Under this form, this result coincides for $\nu = 1$ with the result obtained in Ref. [7] for the asymptotic behavior of the partition of integers with a maximum number of summands (see also [10]).

So far, we have derived two distinct behaviors of the level density with excitation energy: a stretched-exponential behavior in the quantum-degenerate-gas limit, and a power-law behavior in the high temperature classical limit. In the classical limit, in any typical configuration of energy E all the particles of the gas are excited, while in the quantum-degenerate case only a finite fraction of the total number of particles contribute to the excitation energy (the remaining particles are in the ground state). To have a better understanding, in the latter case, of the distribution of the number of excited particles among all the configurations of energy E, and to gain some insight about the transition between the two extreme regimes, we now compute, starting from the degenerate-gas limit $z \to 1$, finite N corrections.

We are interested, in particular, in computing the relative density $F(E, N) = \rho_{\rm MB}(E, N)/\rho_{\rm MB}(E, \infty)$. This quantity gives, among all the possible states of energy between E and $E + dE$, the fraction of those whose number of excited particles does not exceed N. Interestingly, we find three distinct behaviors for $F(E, N)$, depending on the value of ν. In terms of a suitable rescaled variable x that depends on N, E and ν (cf below), the fraction $F(E, N)$ behaves as

$$\nu = 1{:}\ F(E, N) = \exp[-\exp(-x)], \quad (18)$$

$$0 < \nu < 1{:}\ F(E, N) = \begin{cases} 0 & x \leq 0 \\ \exp[-x^{-\nu/(1-\nu)}] & x > 0 \end{cases} \quad (19)$$

$$\nu > 1{:}\ F(E, N) = \begin{cases} \exp(-|x|^\gamma) & x \leq 0 \\ 1 & x > 0. \end{cases} \quad (20)$$

In the latter case, the index γ depends on the precise value of ν [see Eq. (23)]. These three distributions are known as the Gumbel, Weibull, and Fréchet distributions, respectively. They are the three universal limit distributions well known in the theory of extreme value statistics of uncorrelated random variables [3]. Below we outline the main steps in the derivation of Eqs. (18)–(20) and define the rescaled variable x (details will be published elsewhere).

To prove Eqs. (18)–(20) one needs to compute from Eqs. (11) and (12) $\alpha(E, N)$ and $\beta(E, N)$, and to replace them in the expression (10). This is done for large but finite values of the particle number N, i.e., in the limit $z = e^{-\eta} \to 1$, where $\eta = -\alpha$ is a small positive parameter.

Case I: $\nu = 1$.—We find that the appropriate scaling variable for the limiting distribution Eq. (18) is

$$\nu = 1{:}\ x = \beta_1 N + \log\beta_1, \quad (21)$$

where $\beta_1 = (\pi^2/6E)^{1/2}$ was defined in Eq. (14). It follows from Eq. (18) that the asymptotic value for the typical number of excited bosons for states of energy E is $\beta_1^{-1} \log\beta_1^{-1}$.

Case II: $0<\nu<1$.—From the procedure described above, now we obtain for $F(E,N)$ the Fréchet distribution, Eq. (19), with the rescaled variable given by

$$0<\nu<1:\ x=\frac{N}{c_\nu E^{1/(1+\nu)}}, \tag{22}$$

where $c_\nu=[(1-\nu)/\nu]^{(1-\nu)/\nu}[\Gamma(1+\nu)\Gamma(1-\nu)]^{1/\nu}/\theta_\nu^{1/(1+\nu)}$. Note that in Eq. (19) the exponent $\nu/(1-\nu)$ is positive in the corresponding range of ν. This distribution implies that the typical number of excited bosons for states of energy E is $c_\nu E^{1/(1+\nu)}/2$. However, note that the distribution is strongly asymmetric, with a power-law decay (toward 1) for N much larger than the typical value.

Case III: $\nu>1$.—This case is slightly more complicated than the previous ones, because of the presence of a phase transition. In contrast with the previous cases, as N increases and $z\to1$ in Eq. (11) at fixed β, the function $\mathrm{Li}_\nu(z)$ tends to a finite value. At constant temperature, there is thus a critical number $N_c=\Gamma(1+\nu)\zeta(\nu)/\beta^\nu$ of bosons that can be hosted by the thermal cloud, above which a Bose-Einstein condensation starts. We find that the relevant variable in this case is not N but the difference $N-N_c$. The behavior of the distribution is different according to whether N is smaller or larger than N_c. When $N\le N_c$, the exponent γ and the rescaled variable x in Eq. (20) depend on the precise value of ν. Three different regimes are found, summarized as follows

$$1<\nu<2:\ \gamma=\frac{\nu}{\nu-1};\quad x=\frac{\beta_\nu(N-N_c)}{[\nu\Gamma(\nu-1)\Gamma(2-\nu)]^{1/\nu}}, \tag{23}$$

$$\nu=2:\ \gamma=2;\qquad x=\left\{\frac{\beta_\nu^\nu/\nu}{\log[(\beta_\nu^\nu(N_c-N)/\nu)]}\right\}^{1/2}(N-N_c), \tag{24}$$

$$\nu>2:\ \gamma=2;\qquad x=\frac{\beta_\nu^{\nu/2}(N-N_c)}{[\Gamma(\nu+1)\zeta(\nu-1)]^{1/2}}, \tag{25}$$

where β_ν is given in Eq. (14). Finally, for any $\nu>1$ and $N>N_c$ (that corresponds to $x>0$), a macroscopic fraction of the particles is in the ground state. These particles do not contribute to the excitation energy, and their precise number is unimportant. The behavior of the system is thus identical to that of the $N\to\infty$ limit, implying $F(E,N)=1$ for $N>N_c$ (or $x>0$). This completes the demonstration of the Weibull distribution, Eq. (20).

The connection to the number partitioning problem becomes evident if one chooses $\epsilon_j=j$ and E to be a positive integer. The relation $E=\sum_{j=1}^\infty n_j j$ then corresponds to partitioning E into nonzero integers and $N_{\mathrm{ex}}=\sum_{j=1}^\infty n_j$ corresponds to the number of terms or summands in a given configuration of partition. The ratio $F(E,N)=\rho_{\mathrm{MB}}(E,N)/\rho_{\mathrm{MB}}(E,\infty)$ then represents the probability that the number of summands in a random partition of integer E is less than or equal to N. The corresponding limiting Gumbel law for $F(E,N)$ was first proved by Erdös and Lehner by rigorous methods [10]. Our results provide a generalization of this theorem to an arbitrary set of summands characterized by the growth law Eq. (9). The particular case $\epsilon_j=j^s$ with $s>0$ corresponds to partitioning an integer E into sums of sth powers of nonzero integers. For example, for $s=2$, the integer 5 can be partitioned into sums of squares as $5=2^2+1^2=1^2+1^2+1^2+1^2+1^2$. We have shown that while for $s=1$ we recover the Gumbel law, the limiting distribution of $F(E,N)$ is Fréchet for $s>1$ (or $0<\nu<1$) and Weibull for $s<1$ (or $\nu>1$).

In conclusion, we have shown that the density of states of a system of independent bosons is described in a suitable scaling limit by the three limiting laws of extreme value theory. This result has a universal character since it depends only on a single parameter ν that governs the large energy asymptotic average behavior of the SP energy spectrum (and is independent, for instance, of the fluctuation properties of the SP spectrum).

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[1] Y. Alhassid, G. F. Bertsch, S. Liu, and H. Nakada, Phys. Rev. Lett. **84**, 4313 (2000); Y. Kalmykov *et al.*, Phys. Rev. Lett. **96**, 012502 (2006); P. Leboeuf and J. Roccia, Phys. Rev. Lett. **97**, 010401 (2006).
[2] P. Leboeuf, A. G. Monastra, and A. Relaño, Phys. Rev. Lett. **94**, 102502 (2005).
[3] E. J. Gumbel, *Statistics of Extremes* (Columbia University, New York, 1958).
[4] J.-P. Bouchaud and M. Mezard, J. Phys. A **30**, 7997 (1997); D. S. Dean and S. N. Majumdar, Phys. Rev. E **64**, 046121 (2001); G. Gyorgyi, P. C. W. Holdsworth, B. Portelli, and Z. Racz, Phys. Rev. E **68**, 056116 (2003); S. N. Majumdar and P. L. Krapivsky, Physica (Amsterdam) **318A**, 161 (2003); Z. Racz, Proc. SPIE Int. Soc. Opt. Eng. **5112**, 248 (2003).
[5] V. Gritsev *et al.*, Nature Phys. **2**, 705 (2006).
[6] A. Dabholkar, Phys. Rev. Lett. **94**, 241301 (2005).
[7] C. van Lier and G. E. Uhlenbeck, Physica (Amsterdam) **4**, 531 (1937).
[8] C. Weiss and M. Holthaus, Europhys. Lett. **59**, 486 (2002); A. M. Vershik, Funct. Anal. Appl. **30**, 90 (1996).
[9] G. E. Andrews, *The Theory of Partitions* (Cambridge University Press, Cambridge, England, 1998).
[10] P. Erdös and J. Lehner, Duke Math. J. **8**, 335 (1941).
[11] F. C. Auluck and D. S. Kothari, Proc. Cambridge Philos. Soc. **42**, 272 (1946).
[12] C. B. Haselgrove and H. N. V. Temperley, Proc. Cambridge Philos. Soc. **50**, 225 (1954).
[13] G. H. Hardy and S. Ramanujan, Proc. London Math. Soc. **17**, 75 (1918).
[14] B. K. Agarwala and F. C. Auluck, Proc. Cambridge Philos. Soc. **47**, 207 (1951); see also M. N. Tran, M. Murthy, and R. K. Bhaduri, Ann. Phys. (N.Y.) **311**, 204 (2004).
[15] H. M. Sommermann and H. A. Weidenmüller, Europhys. Lett. **23**, 79 (1993).